Abstract Submitted to the
International Conference on Strongly Correlated Electron Systems
University of Michigan, Ann Arbor
August 6-10, 2001

Electronic structure and structural properties of elemental plutonium

Nicholas Kioussis[1], P. Turchi and A. Gonis[2], D. Price[3], B. R. Cooper[4]

[1] *California State University, Northridge, Northridge, CA 91330, USA*
[2] *Lawrence Livermore National Laboratory, Livermore, CA 94551, USA*
[3] *University of Memphis, Memphis, TN 38152, USA*
[4] *West Virginia University, Morgantown, WV 26506, USA*

Electronic structure calculations, based on the full-potential linear muffin tin orbital method, have been used to study the ground-state and structural properties of the α phase (monoclinic) and δ phase (fcc) of elemental plutonium. In order to investigate the effect of the electron-electron correlations on the equilibrium properties, we have employed electronic structure calculations based on density functional theory within the local density approximation (LDA), a constrained version of the LDA in which the f-electrons are confined to core states, and finally the so-called LDA+U method. The Coulomb interaction parameter U is calculated as a function of volume on a wholly $ab\ initio$ basis. The LDA fails to provide an accurate description of the electronic structure and related properties. Some improvement can derive from constrained LDA calculations and from the application of the LDA+U method. However, the former of these leads to an unacceptably large ground-state energy, while all approaches fail to yield the experimentally observed $\delta \rightarrow \alpha$ volume collapse. Detailed information from the calculations will be presented, such as total energies as function of volume, density of states, and charge-density contour plots.
Supported by NSF DMR-95310005